Session: Major Efforts in Nonequilibrium Flows (Invited)

9:00 AM-9:30 AM	**Oral Presentation. Modeling, Measurements, and Fundamental Database Development for Nonequilibrium Hypersonic Aerothermodynamics** *D. Bose*
9:30 AM-10:00 AM	**AIAA-2012-0724. Nonequilibrium Processes in Hypervelocity Flows: An Analysis of Current Modeling Approaches** *G. V. Candler*
10:00 AM-10:30 AM	**AIAA-2012-0725. Review of the VKI research on nonequilibrium phenomena in hypersonics** *T. E. Magin; O. Chazot*
10:30 AM-11:00 AM	**Oral Presentation. High-Speed Flow Studies at ITAM** *M. S. Ivanov; A. Maslov; Y. Bondar*
11:00 AM-11:30 AM	**Oral Presentation. Review of Experimental Studies Being Conducted in LENS Shock and Expansion Tunnels to Evaluate the Characteristics of Real Gas and Plasma Flows** *M. S. Holden; M. G. MacLean; R. A. Parker; T. P. Wadhams*
11:30 AM-12:00 PM	**AIAA-2012-0726. Study of hypervelocity non equilibrium flows in impulse facilities** *R. G. Morgan*

Modeling, Measurements, and Fundamental Database Development for Nonequilibrium Hypersonic Aerothermodynamics

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50th AIAA Aerospace Sciences Meeting, Jan 09-12, 2012

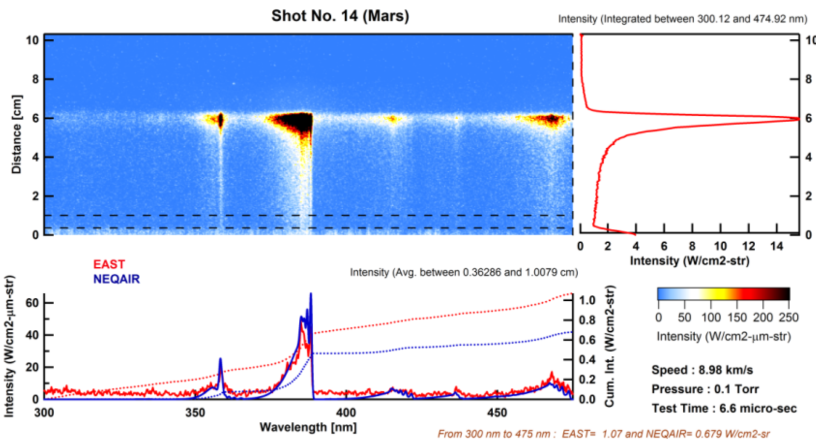
Acknowledgements

- Aaron Brandis, Brett Cruden, Dinesh Prabhu, Rich Jaffe (NASA Ames)
- Alan Wray, Yen Liu, Galina Chaban, David Schwenke, Duane Carbon (NASA Ames)
- Chris Johnston, Artem Dyakonov (NASA Langley)
- Winifred Huo (Huo Consulting)
- Prof. Doug Fletcher (University of Vermont)
- Matt MacLean (CUBRC)

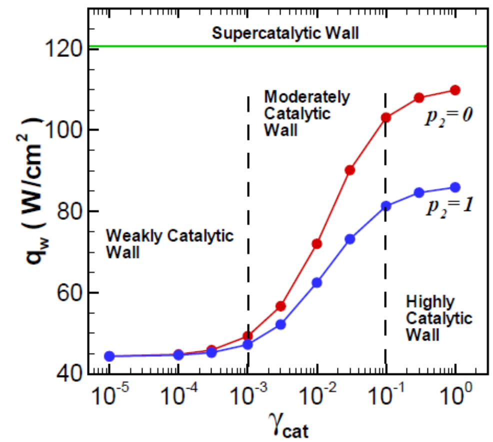
Nonequilibrium Phenomena in Hypersonic Flow

- **Nonequilibrium occurs when time scales of thermochemical processes are longer than fluid transport time scale**
- **Nonequilibrium conditions generally occur in low pressure environment and/or in flows with high gradients**
- **Nonequilibrium phenomena occurs**
  – in shock wave
  – in boundary layer
  – on surfaces (catalycity, ablation)
  – in expanding flow (nozzles, plumes, wakes, etc.)

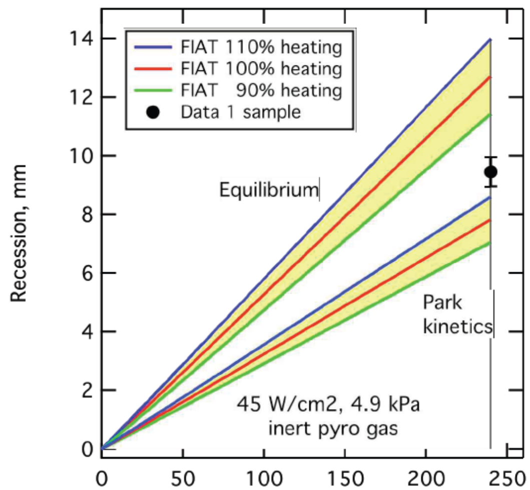
Impact of Nonequilibrium Phenomena



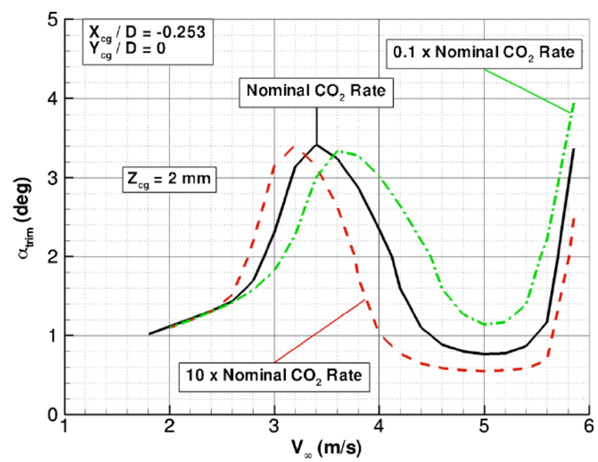
Radiative Heating: Nonequilibrium radiation can be several fold larger than equilibrium radiation



Convective Heating: Wall catalycity can raise aeroheating by several factors

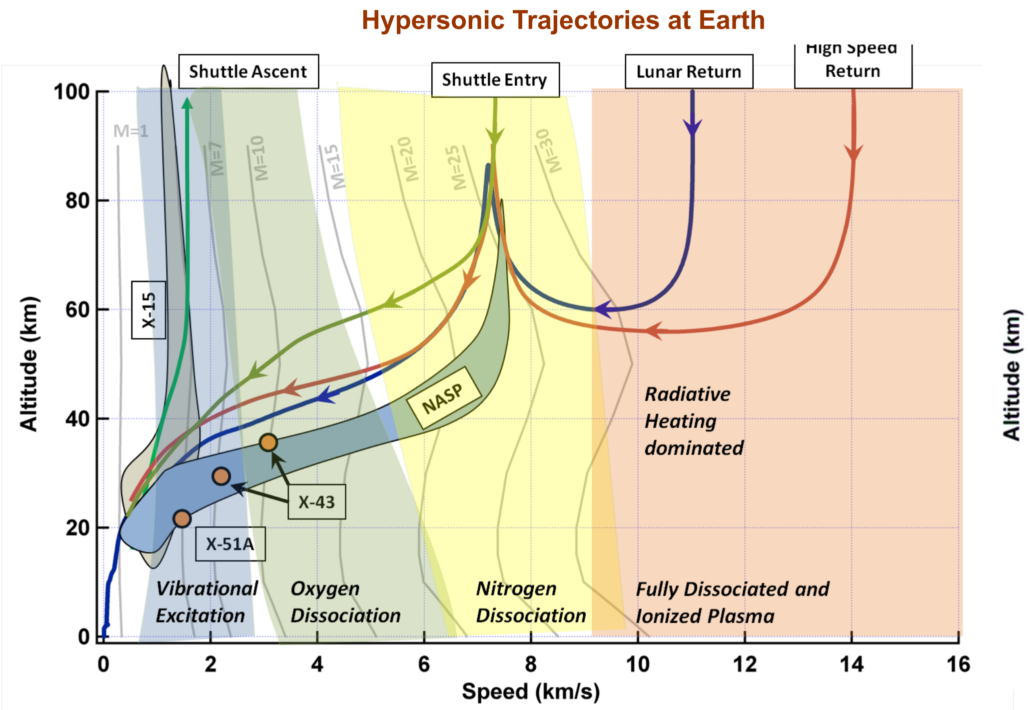


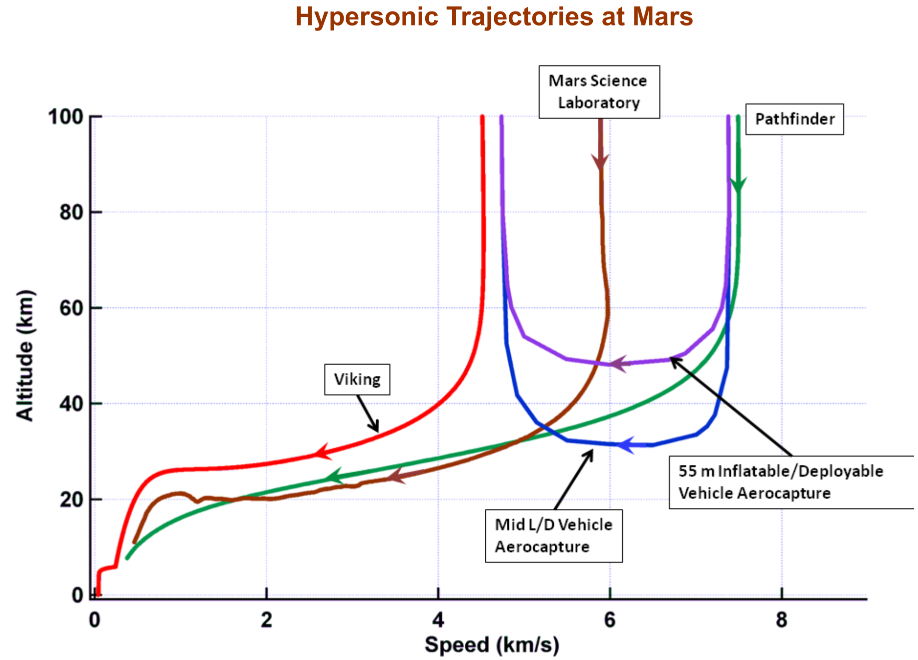
Ablation: Nonequilibrium oxidation can significantly reduce recession



Aerodynamics: Nonequilibrium can alter trim angles by over 1-deg

Nonequilibrium Thermochemical Phenomena in Flight





- Nonequilibrium phenomena exists at all flight regimes, however, its impact is dependent on flow enthalpy, vehicle size, pressure, etc.
- In the upper right of the figures, nonequilibrium phenomena is driven by nonequilibrium ionization and non-Boltzmann kinetics
- Nonequilibrium can be important in the lower left part of the figure as well where it affects shock shapes and vehicle aerodynamics

NASA Research Activities in Nonequilibrium

Fundamental Database

- Atomic Spectra
- Diatomic Spectra
- Triatomic Spectra
- Energy Transfer
- Reaction Cross Sections
- Electron Impact Cross Sections
- Radiative Processes

Measurements

- Shock Tube Measurements
- High Enthalpy AerothermalTesting
- Gas-Surface Interactions
- MSL Entry Flight Instrumentation
- Arcjet Testing for Ablation
- Facility Characterization and Diagnostics

Modeling

- HyperRad Code
- Mars Chemistry
- Non-Boltzmann Excitation
- VUV Radiation
- Generalized Gas-Surface Interaction
- Nonequilibrium Ablation
- DSMC

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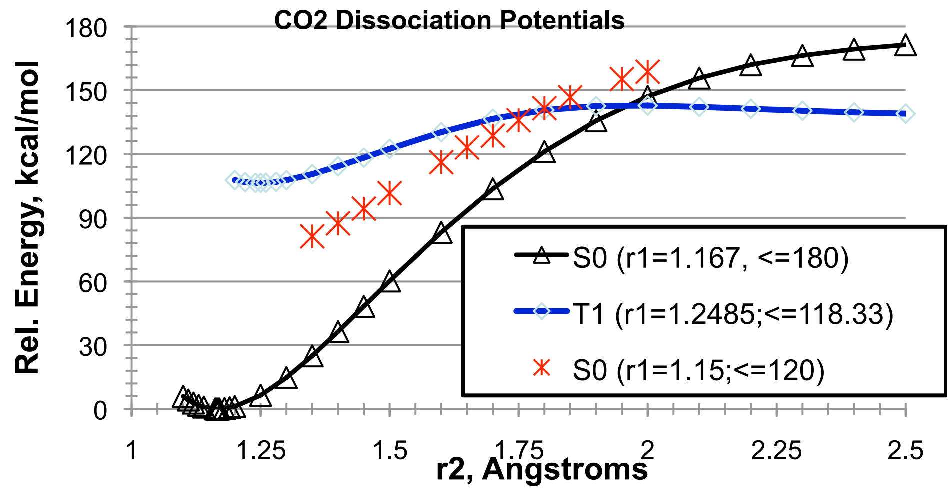
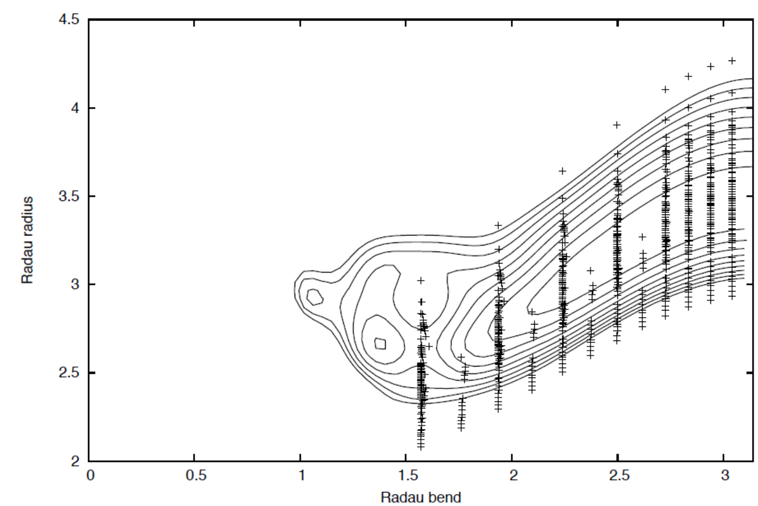
Ab-initio Computations of Triatomic Potentials

- **CO_2 Excitation & Dissociation:**
  - A critical process with impact on re-entry aerodynamics, IR radiation in the wake, freestream kinetics in high enthalpy tunnels
  - It is likely that CO2 singlet → triplet transition is the bottleneck in CO2 dissociation; its rate is being determined to describe CO2 dissociation and recombination process
- **C_3 and C_2H Potentials:**
  - Key ablation products in boundary layer that significantly absorb incident shock layer radiation
  - C_3 Potential energy surfaces for two key transitions that absorb radiation are being characterized
    - Swings system ($X^1\Sigma_g^+ \rightarrow A^1\Pi u$): near UV 300-430 nm
    - ($^1\Sigma_g^+ \rightarrow {}^1\Sigma_u^+$): VUV transition 140-190 nm

Content provided by Rich Jaffe (NASA Ames)



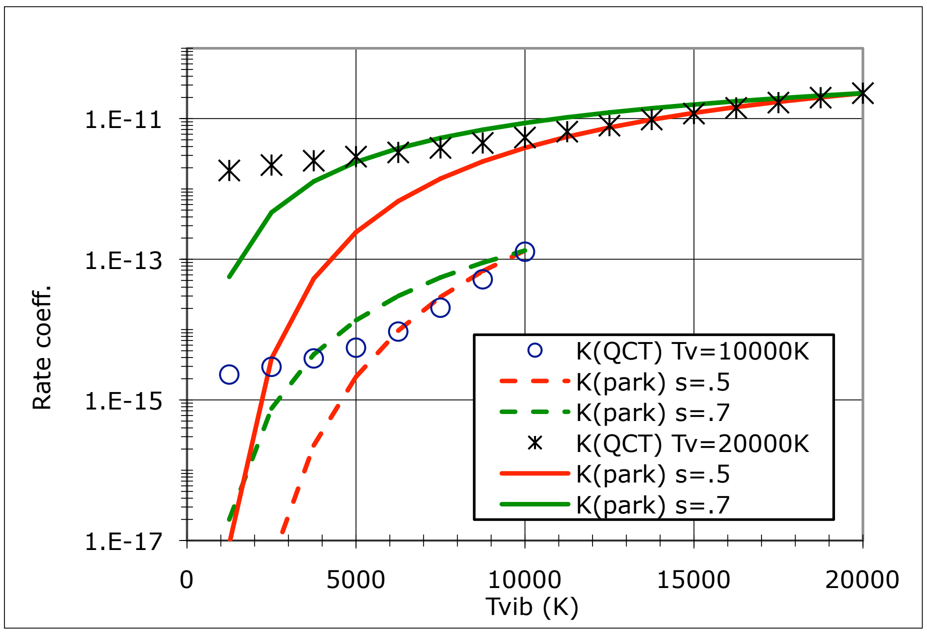
Singlet and Triplet CO2 Dissociation Potentials



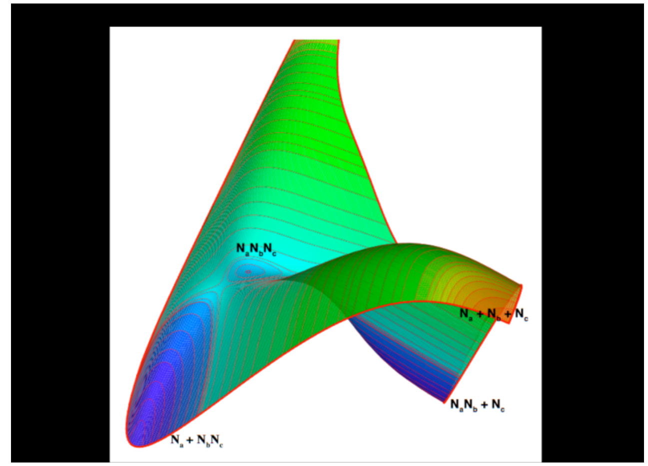
Ground State $C3(X^1\Sigma_g^+)$ Potential Energy Surface

N_2 Collisional Energy Transfer and Dissociation

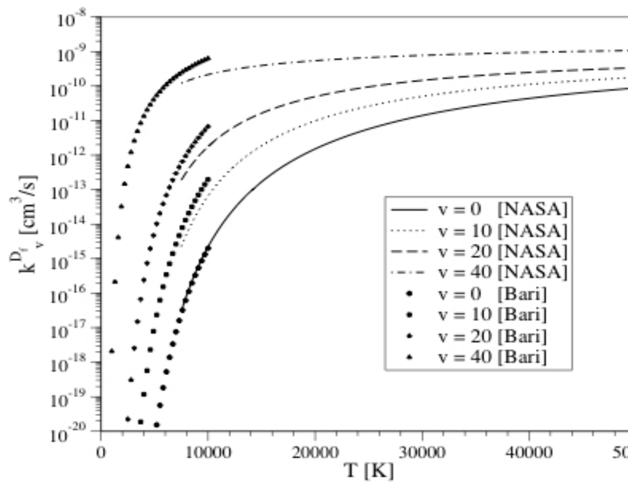
- **State-Specific Cross Sections**
  - Ab-inito potential energy surfaces generated for N_2+N and N_2+N_2 systems
  - Energy transfer and dissociation cross sections determined for binned ro-vibrational energies



Evaluation of Park's *TTv* Vibration-Dissociation Model



N_2+N Potential Energy Surface



Vibrational State-Specific Reaction Rate Quasi Classical Trajectories

Content provided by Rich Jaffe (NASA Ames)

Electron Impact Excitation and Ionization

- **Nonequilibrium Electronic Excitation and Ionization:**
  - In low pressure flight regimes (occurs in Mars, Titan, and Earth entry), the electronic states of radiating species do not reach a Boltzmann equilibrium, and generally reduce radiation by a factor 2 or more.
  - A nonequilibrium model requires a collisional-radiative or a QSS (quasi steady state) model
- **Ab-Initio Cross Sections:**
  - Electron Impact Reactions:

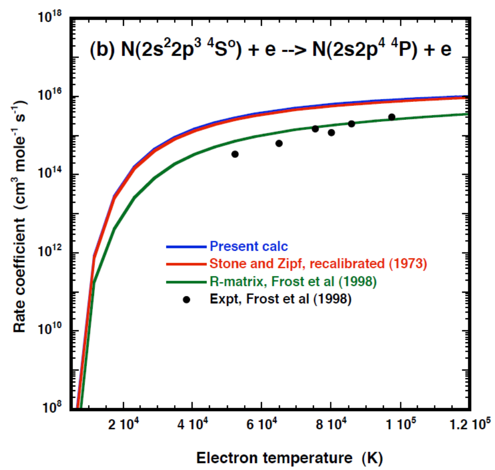
$$e + M(X) \Leftrightarrow e + M(A)$$

$$e + M \Leftrightarrow M^{+} + 2e$$

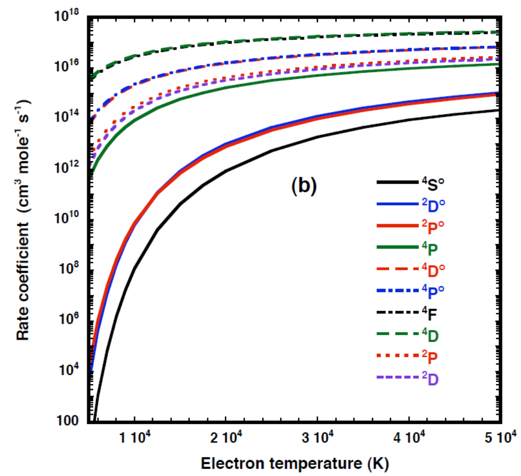
  - Photoionization and radiative recombination

$$e + M^{+} \Leftrightarrow M + h\nu$$

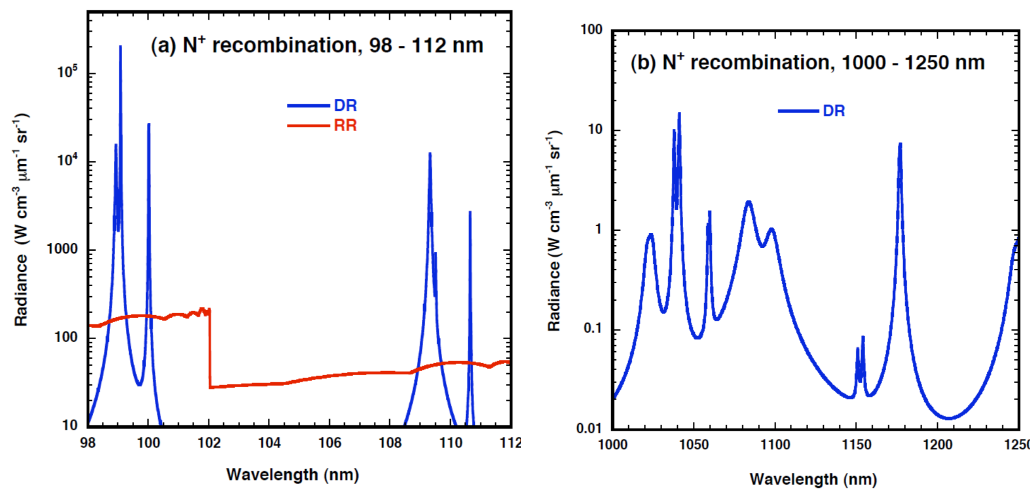
$$M : N, N_2, O$$



Electron Impact Excitation Rates of Atomic N



Electron Impact Ionization Rates of Atomic N



Radiative (RR) and Dielectronic Recombination Spectra

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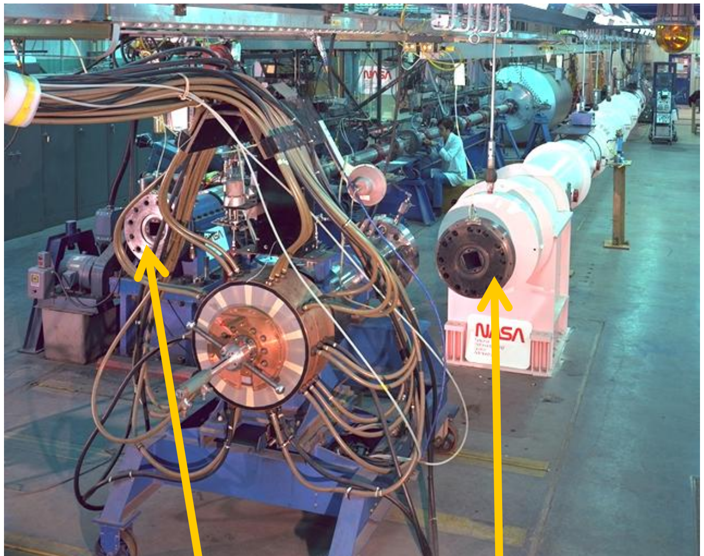
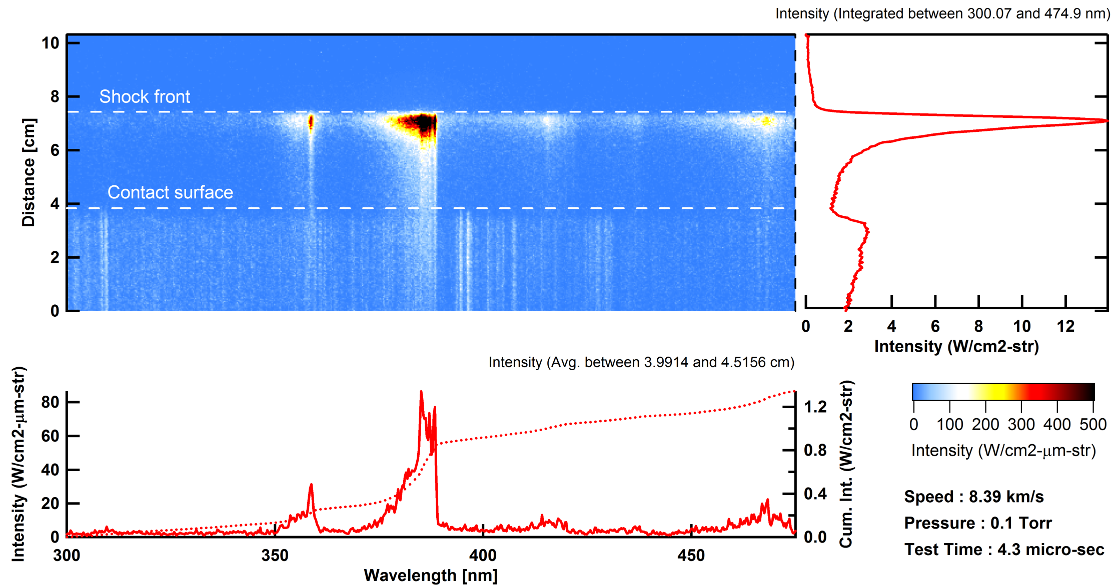
Shock Tube Measurements

NASA Ames Electric Arc Shock Tubes



4-in Operational Shock Tube

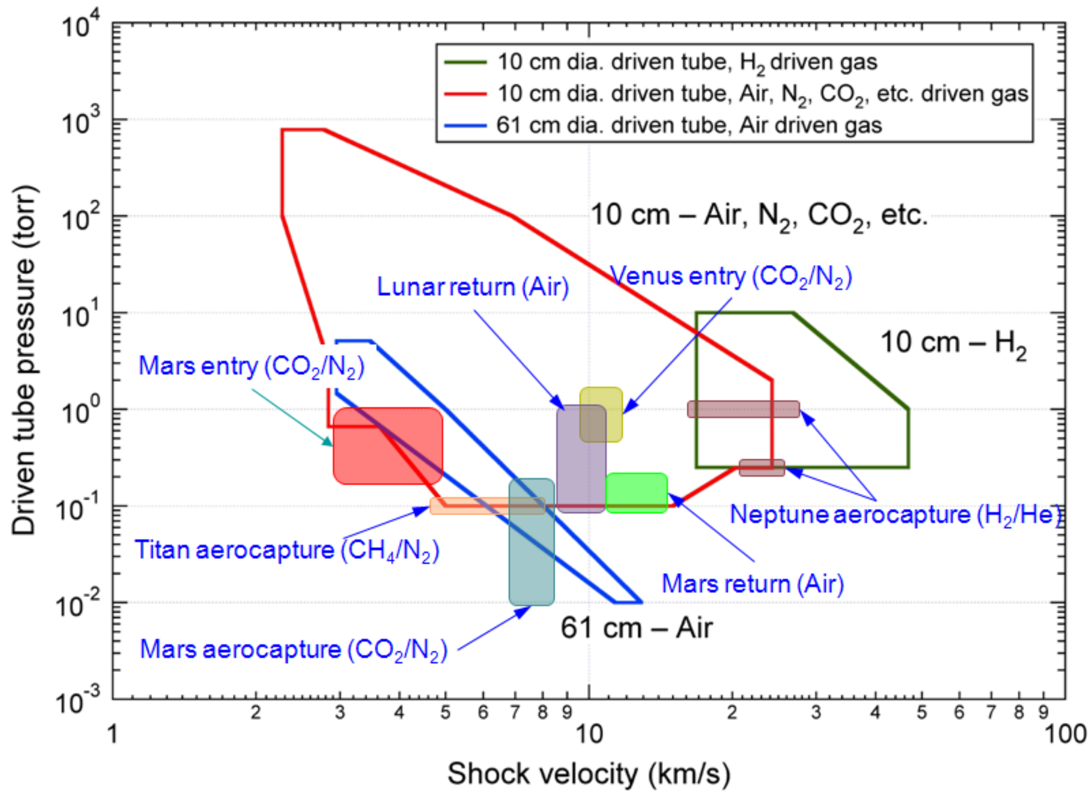
24-in Low Density Shock Tube (being brought online)



Spectrally and Spatially Resolved Quantitative Intensity

- **Developed in the mid 1960s; operational in early 1970s**
- **10.16 cm dia. aluminum driven tube**
- **Unique capabilities**
  - Shock speed range (up to 46 km/s)
  - Driven gas composition
  - Optical instrumentation with calibrated intensity measurements from VUV to mid-wave IR

Flight Relevance

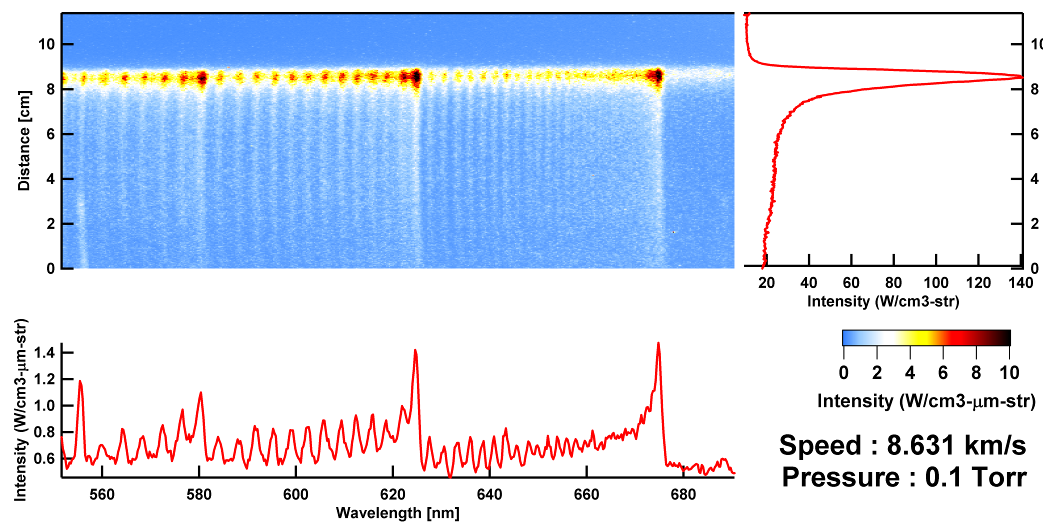


- **Emission measurements made at several planetary entry conditions**
- **~800 images of detailed and quantified emission intensities obtained**
- **Unprecedented levels of model validation underway for both equilibrium and nonequilibrium radiation for Earth and Mars entry**
  - **Mars entry radiation is dominated by nonequilibrium phenomena**

Figure provided by Brett Cruden (ERC-NASA Ames)

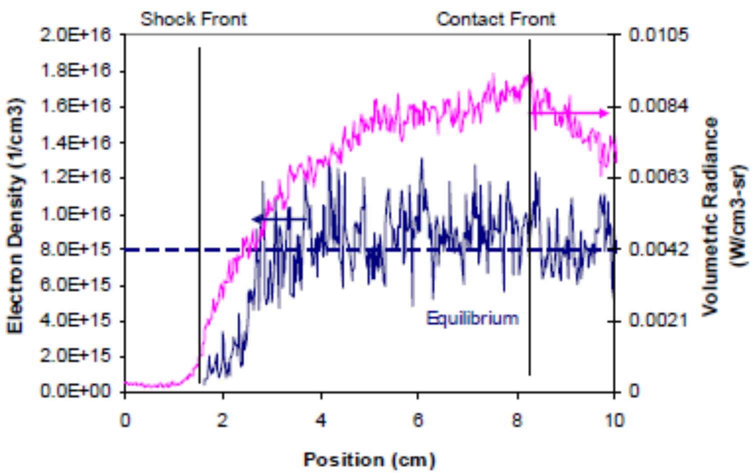
Nonequilibrium Relaxation

- Emission measurements made at Earth and Mars entry conditions
- ~800 images of detailed and quantified emission intensities obtained
- Unprecedented levels of model validation possible for both equilibrium and nonequilibrium radiation for Earth and Mars entry



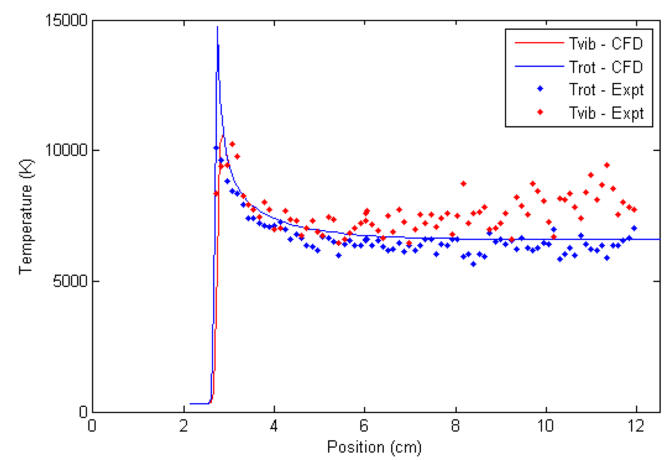
Speed : 8.631 km/s
Pressure : 0.1 Torr

Spectrally and Spatially Resolved Quantitative Intensity



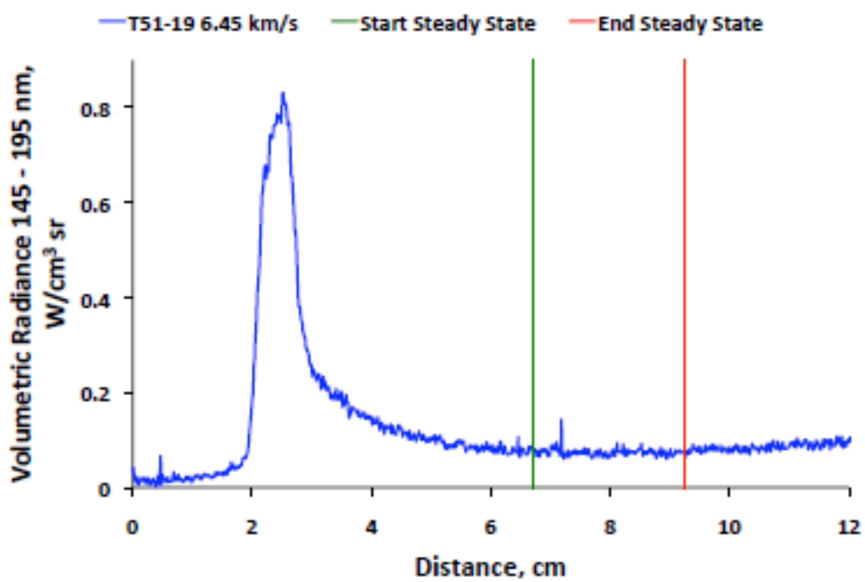
Electron Density Profile Behind a 10 km/s Shock Inferred from Atomic Line Broadening

Figures provided by Brett Cruden (ERC-NASA Ames)

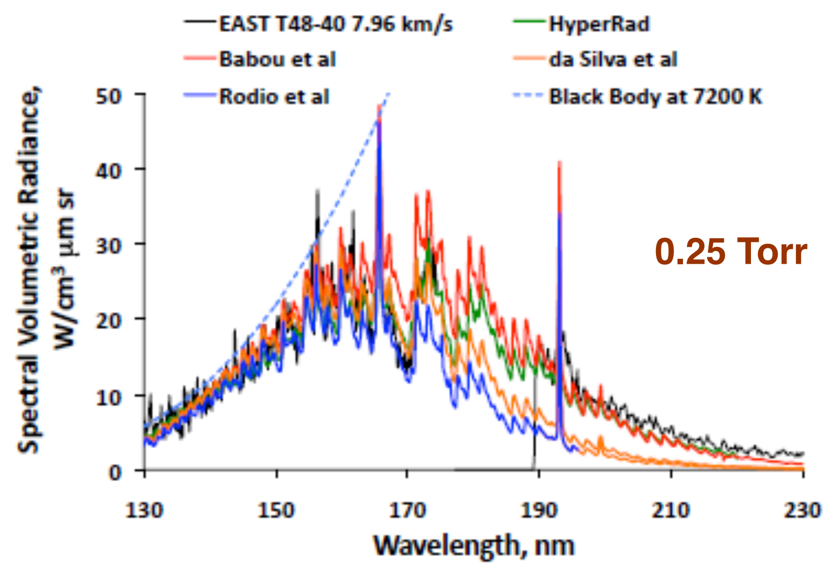


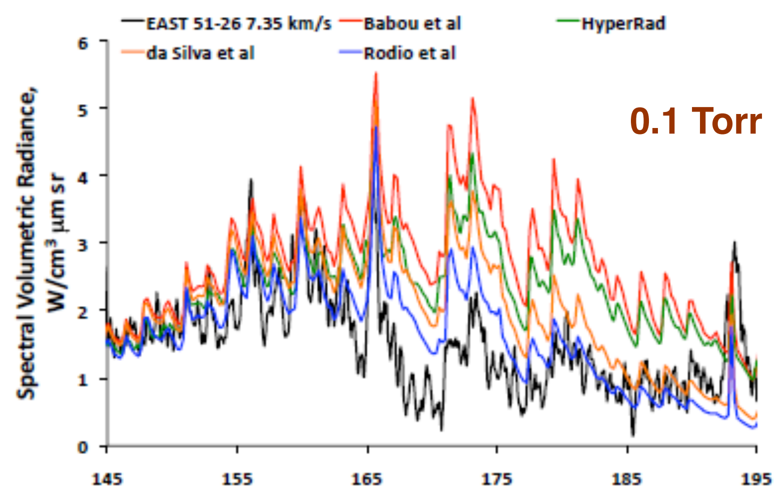
Nonequilibrium Vibrational and Rotational Temperature Profiles Inferred from CN violet Spectrum

CO Fourth Positive Vacuum UV Radiation



CO4+ Intensity Behind a 6.45 km/s, 0.25 Torr Shock



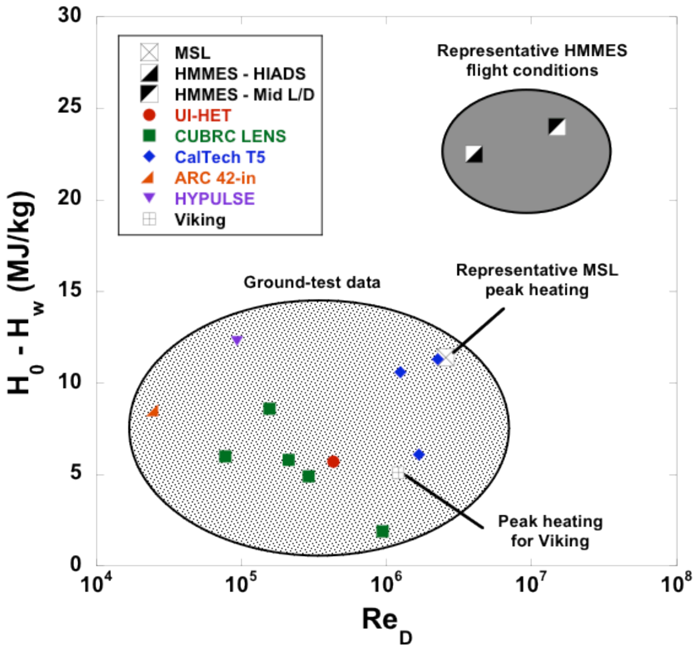


CO4+ Spectral Comparisons with Different Databases

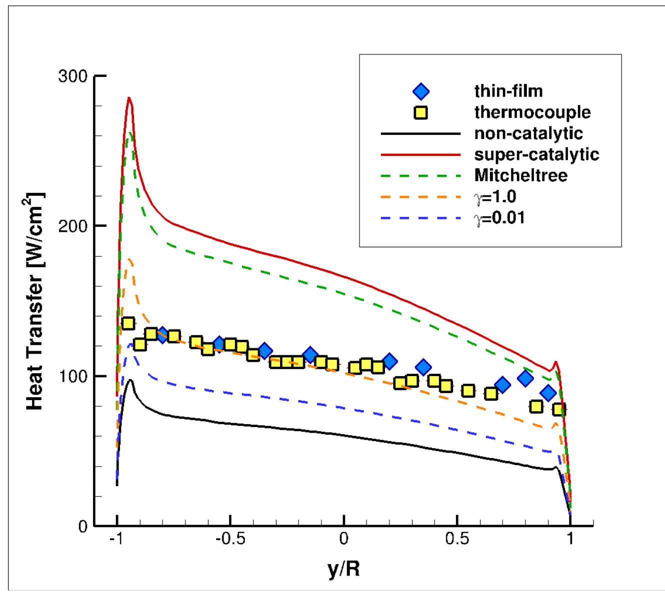
- **VUV radiation dominates radiative heating at high speed entries**
- **CO4+ radiation in the VUV spectrum measured for model validation**
- **Nonequilibrium excited state population at low pressure 0.1 Torr may be responsible for over prediction**

Figures provided by Aaron Brandis (UC-Santa Cruz-NASA Ames)

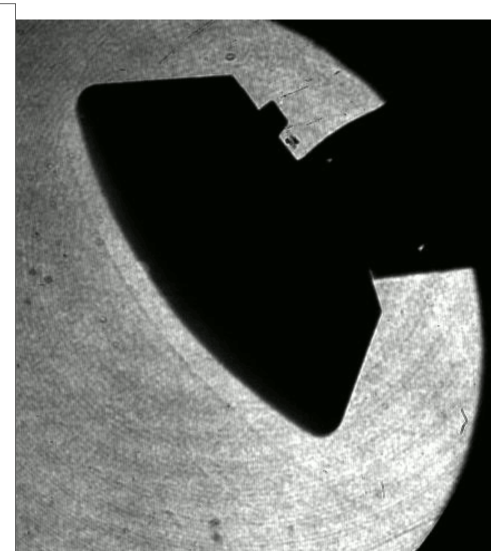
High Enthalpy Aerothermal Measurements



Ground to Flight Traceability of past CO2 High Enthalpy Tests



Heat Transfer Measurements



Schlieren Image

CUBRC LENS-XX Measurements in CO2 at 15.3 MJ/kg, 18-deg AoA,

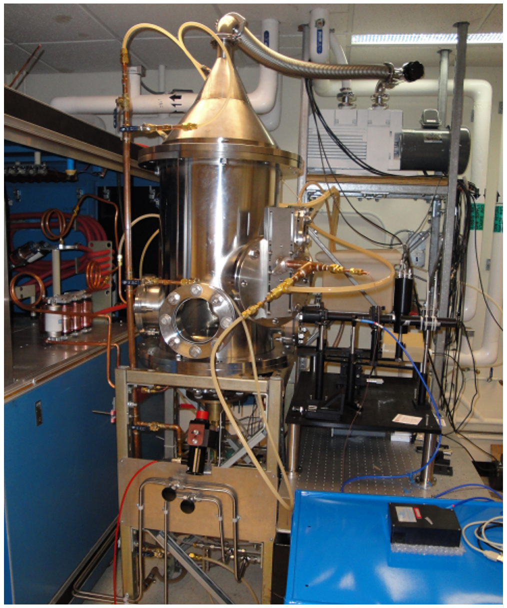
- High enthalpy test campaign underway in CUBRC LENS XX expansion facility with freestream free of nonequilibrium
- High enthalpy aerothermal thermal tests in CO2 environment has enabled validation of
  - CO2 chemistry mechanism and energy transfer
  - Catalycity models

Figures provided by Matt MacLean (CUBRC) and Dinesh Prabhu (ERC-NASA Ames)

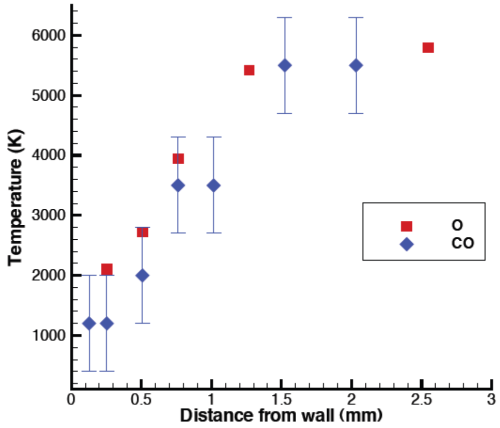
Gas-Surface Interaction Measurements

- Fundamental measurements in reacting boundary layers at flight relevant condition are rare
- University of Vermont (Prof. Doug Fletcher) 30 kW ICP Torch produces subsonic plasma representative of stagnation conditions in flight
- Two-photon LIF measurements of temperature and species density are made in the boundary layer
- Flight materials in CO_2 environment are being evaluated for high mass Mars entry system

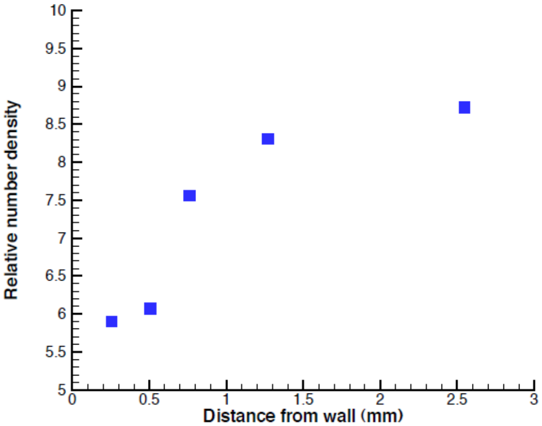
Content provided by Prof. D. Fletcher (University of Vermont)



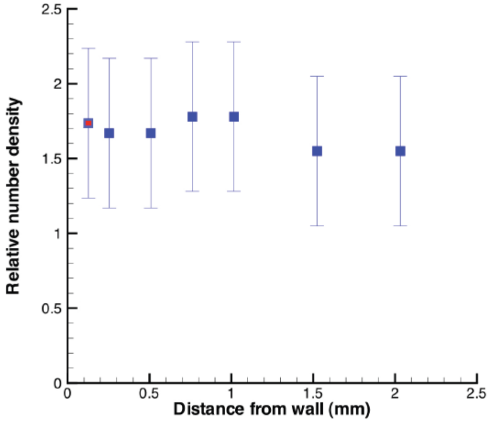
UVM 30kW ICP Facility



Temperature from Scans of O and CO in a CO2/Ar over Graphite

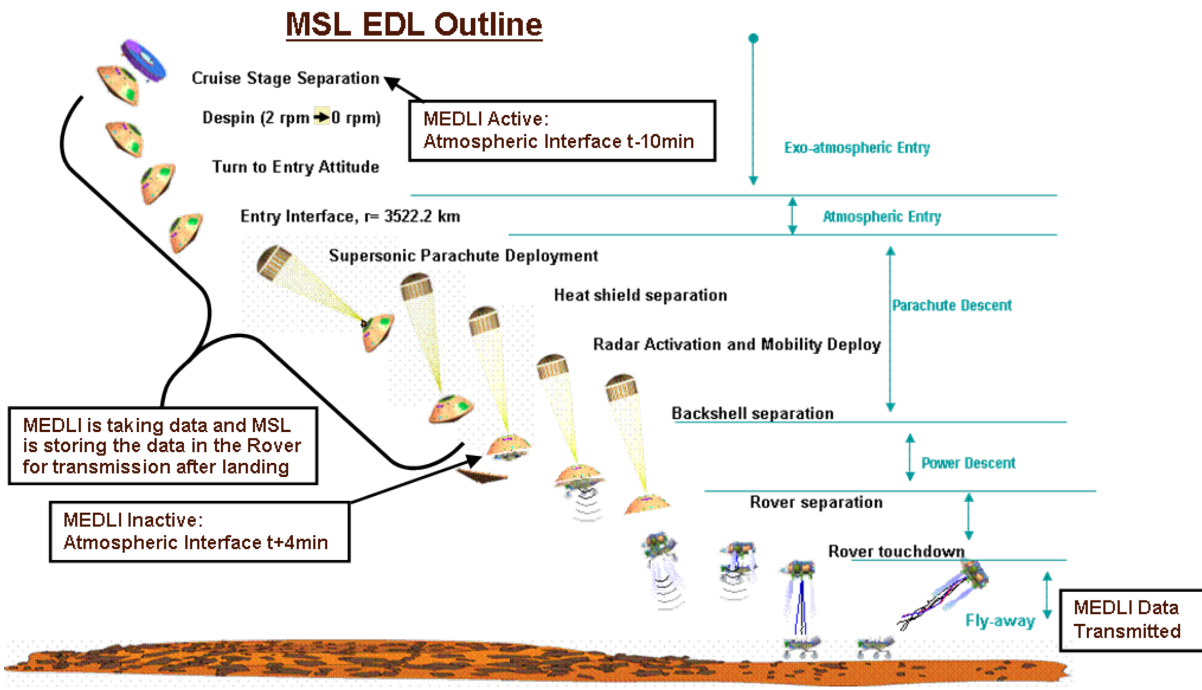


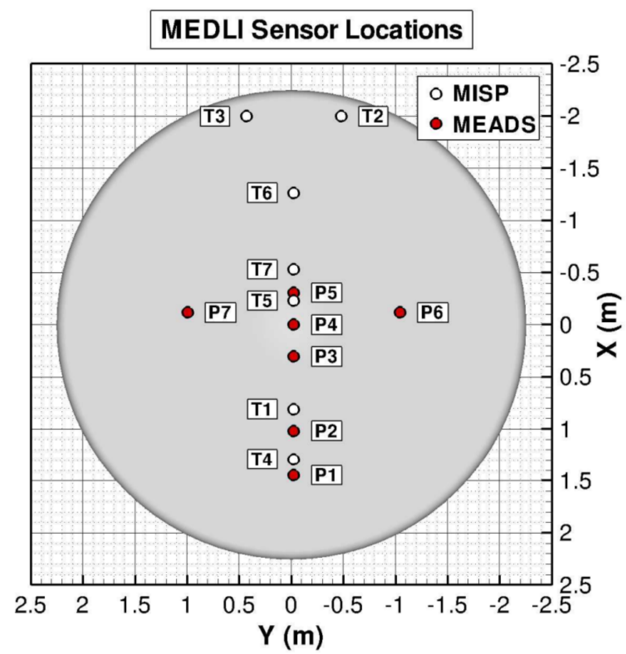
Atomic O Density in CO_2 Plasma over Copper



CO Density in CO_2 Plasma over Copper

Mars Entry Aero/Aerothermal/TPS Response Measurements: MEDLI Project





- Mars Science Laboratory (MSL) heatshield instrumented with thermocouples and pressure sensors (Aug 2012 entry)
- Unprecedented opportunity to obtain flight data at Mars in nonequilibrium flow to validate
  - aerothermal models
  - aerodynamic models
  - ablation models

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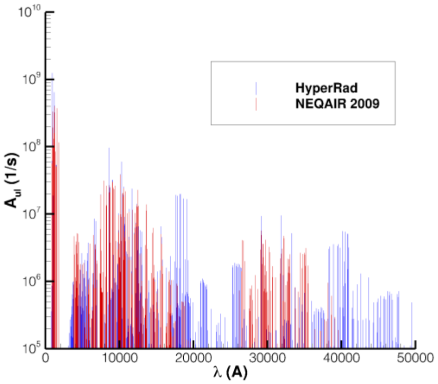
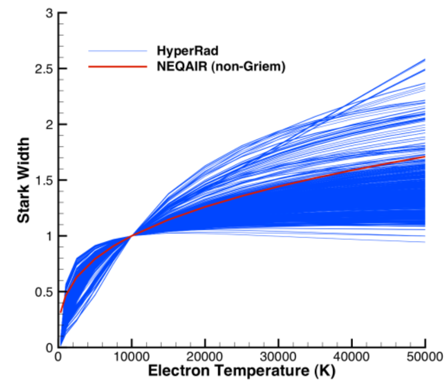
HyperRad Radiation Code

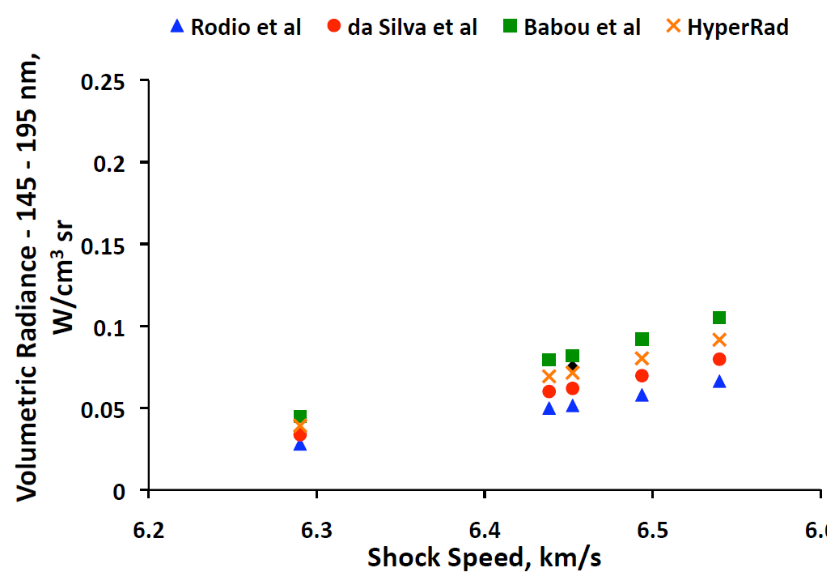
- **HyperRad is a new radiation code reliant on newly developed ab-initio database**
  - Improved atomic lines; almost 5X as many lines as available in 2009 NEQAIR
    - Careful merger of NIST, Vanderbilt, and Top-Base line datasets
  - Improved Stark width and shift database
  - Line list driven molecular databases
  - Improved bound-free radiation routines based on ab initio cross sections
  - Three-dimensional radiation transport
  - Coupled thermal, chemical, and radiation nonequilibrium for excited state populations
  - Designed for high end computing and paralellization
  - First version released in 2011
  - HyperRad Development Team: *Wray, Liu, Schwenke, Chaban, Huo, Carbon, Jaffe (NASA Ames)*



Improved Line Database in HyperRad



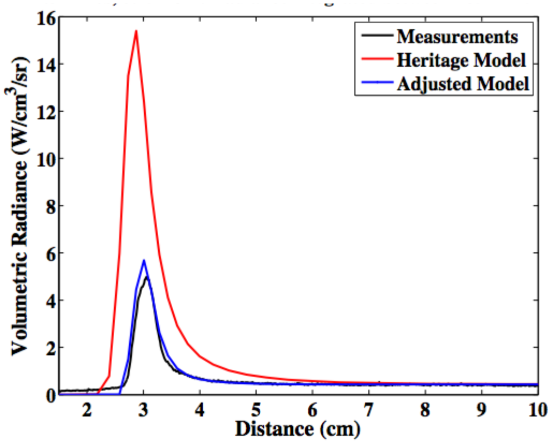
Temperature Dependence of Stark Width



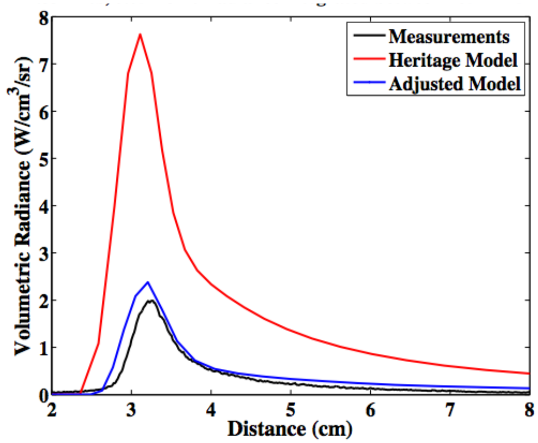
Comparison of various CO4+ databases at 0.25 Torr

Mars Entry Chemical Kinetics Model

7.82 km/s, 0.25 Torr, 165-215 nm

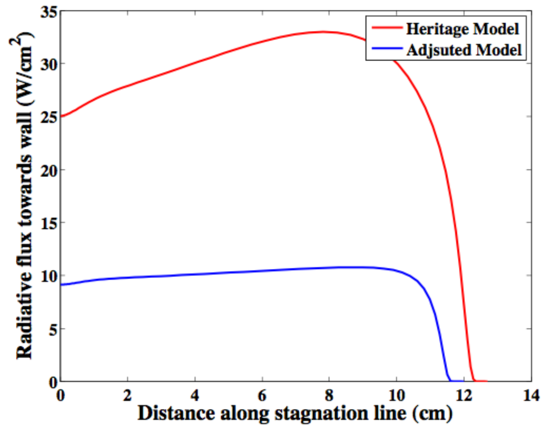


7.82 km/s, 0.05 Torr, 165-215 nm



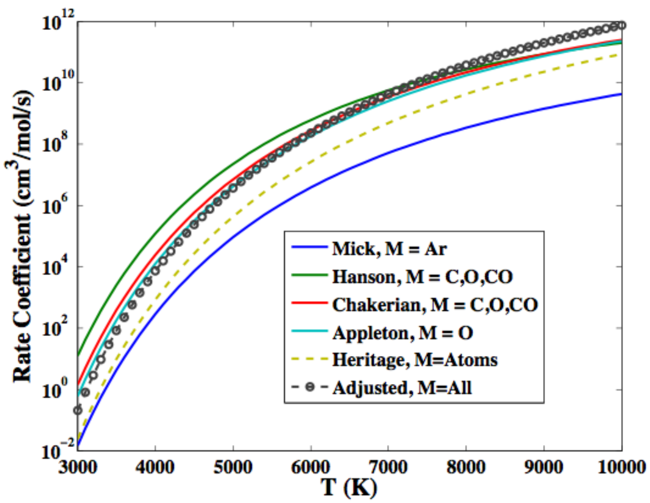
Nonequilibrium Radiation Intensity Compared with Shock Tube Measurements

Wall-directed Radiative Flux



Conditions: 7 km/s, 3X10^{-4} kg/m3, 5m diameter, 60-deg sphere cone

Adjusted Rate of CO Dissociation

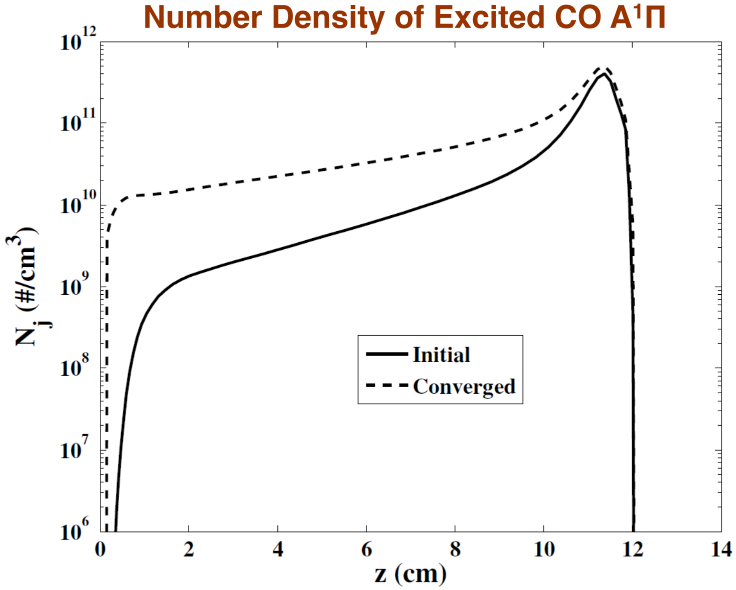


- Currently used Mars entry chemistry mechanism was proposed by Park and co-workers nearly 20 years ago, based on very little measured data
- With detailed shock tube measurements and testing in high enthalpy facilities, it is now possible to significantly improve the chemistry model

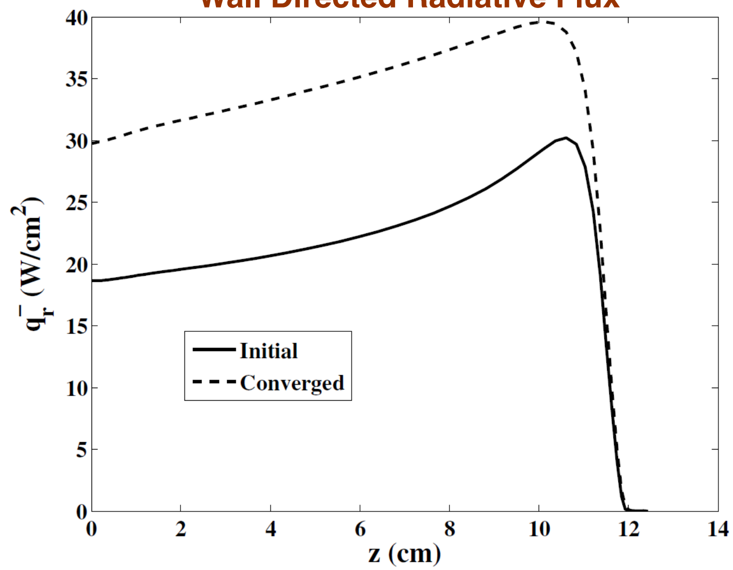
Content provided by Chris Johnston (NASA Langley)

Non-Boltzmann Excitation Modeling

Number Density of Excited CO $A^1\Pi$



Wall Directed Radiative Flux



Profiles along stagnation streamline showing influence of non-local absorption on excited state chemistry and radiation
Conditions: 7 km/s, 10^{-4} kg/m3, 5m diameter, 60-deg sphere cone

Excited State Chemistry Mechanism

1	$CO(X^1\Sigma^+) + M \leftrightarrow CO(A^1\Pi) + M$
2	$CO(a^3\Pi_r) + M \leftrightarrow CO(A^1\Pi) + M$
3	$CO(X^1\Sigma^+) + e^- \leftrightarrow CO(A^1\Pi) + e^-$
4	$CO(X^1\Sigma^+) + e^- \leftrightarrow CO(a^3\Pi_r) + e^-$
5	$CO(a^3\Pi_r) + e^- \leftrightarrow CO(A^1\Pi) + e^-$

- **Non-Boltzmann modeling, integrated with CFD (HARA and LAURA), is being applied to model radiative heating environment on a high mass Mars entry system**
- **Validation data at low pressures to support modeling is expected from Ames 24-in shock tube**

Content provided by Chris Johnston (NASA Langley)

Concluding Remarks

- Modeling of nonequilibrium phenomena is complex and must be supported by experimental measurements and fundamental database development
- Model development based on fundamental physics as well as phenomenological approaches are needed
- While NASA is supporting a wide range of research activities in nonequilibrium phenomena, several key areas lack a critical-mass (e.g. diagnostics development, DSMC, ...)
- NASA research in nonequilibrium phenomena for outer planet entries has languished
- We invite partnerships as much of our data and results can be shared openly

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